



Data updates on Norine, the reference Non-Ribosomal Peptide knowledge base

Yoann Dufresne, Juraj Michalik, Areski Flissi, Valérie Leclère, Maude Pupin

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Data updates on Norine, the reference Non-Ribosomal Peptide knowledge base

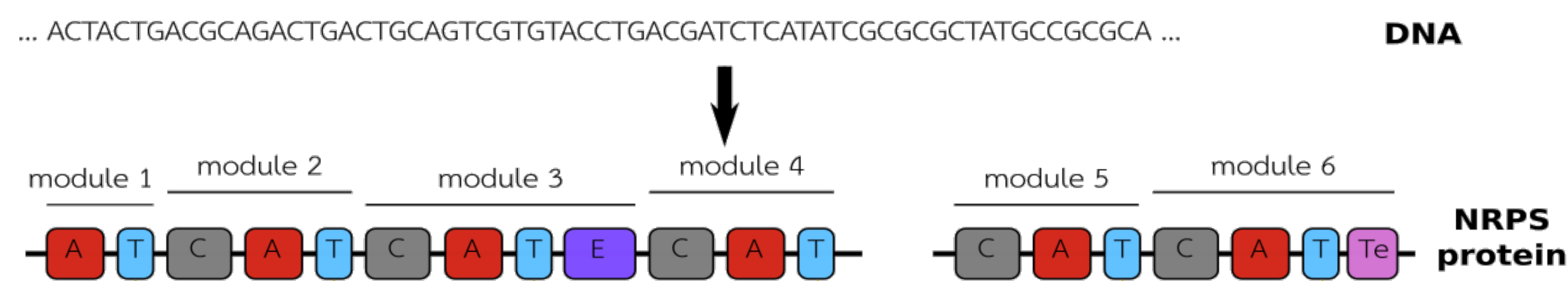
Authors : Yoann Dufresne¹, Juraj Michalik¹, Areski Flissi¹, Valérie Leclère^{1,2}, Maude Pupin¹

¹Laboratoire CRISTAL (UMR CNRS 9189) et centre Inria de Lille Nord-Europe, équipe Bonsai, Université Lille 1

² Institut Charles Viollette, ProBioGEM team, EA 7394, Lille 1

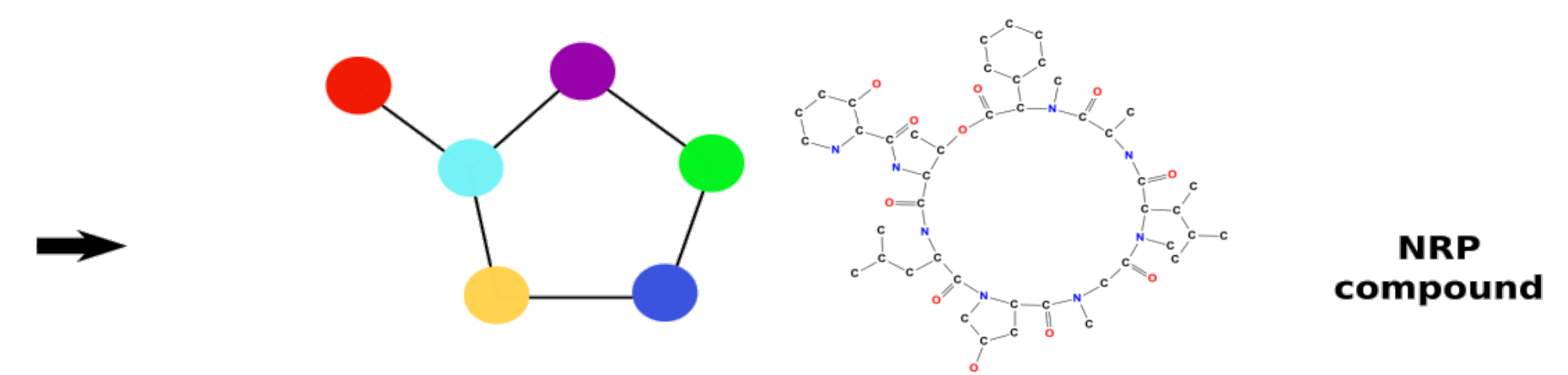
The Nonribosomal Peptides (NRP) pathway

Biological pathway



Non Ribosomal Peptides (NRP) are small polymers synthesised by enzymes. The enzymes (called Non Ribosomal Peptide Synthetases (NRPS)) are modular proteins grouped in complexes that select monomers and create NRP. One complex only creates one kind of NRP. The study of the proteic sequence of NRPS and the analysis of mass spectra led to discover hundreds of these molecules.

Compounds and interest



The NRPs are very interesting because of their particular structures and compositions. They are composed of many different monomers (more than 500) organized in various structure conformations (cycles, branches and mix of them). These particularities lend them many unique interesting activities.

Data update in Norine

Norine V2
1186 NRPs
536 monomers

Norine V2

- Reference knowledge-base for NRPs since 2009
- Manually curated annotations
- Open to expert sourcing by user-friendly forms
- But several NRPs are missing

Third-party databases

Other databases store NRPs, among other molecules

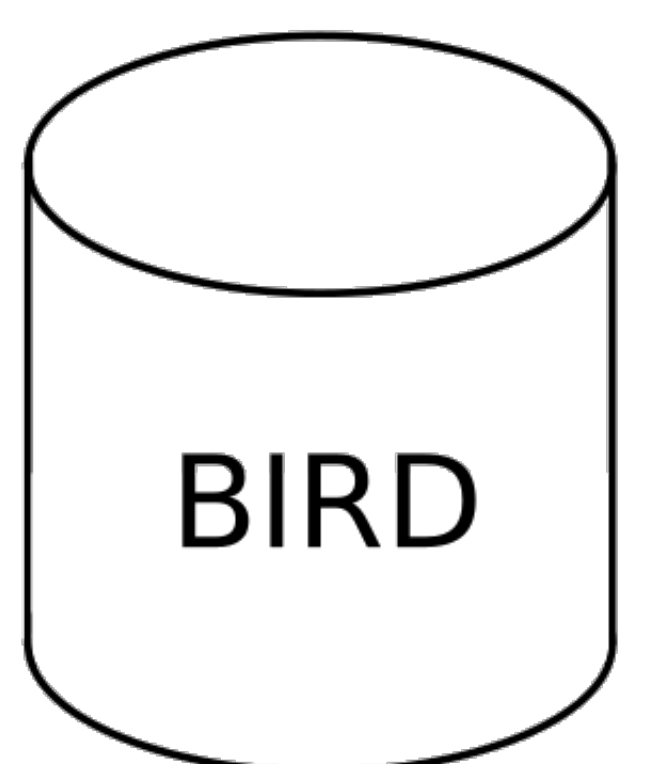


MIBiG

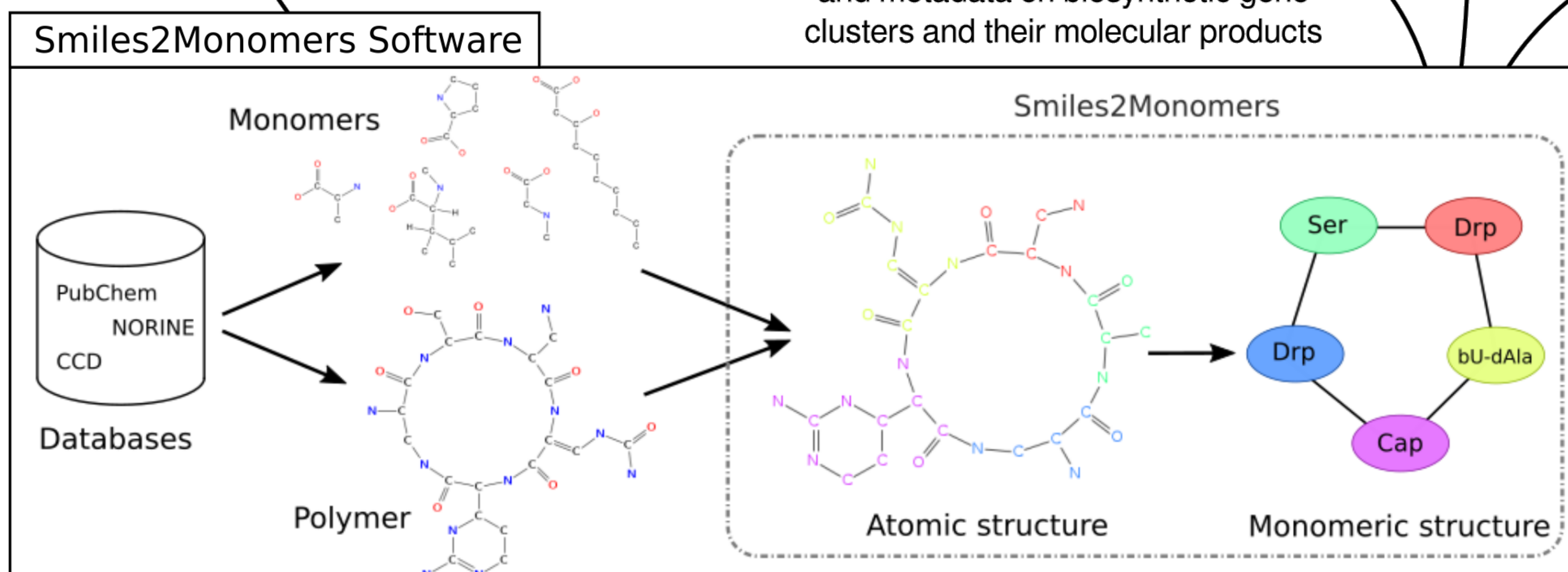
community standard for annotations and metadata on biosynthetic gene clusters and their molecular products



PubChem
Information on the biological activities of small molecules



BIRD (wwPDB)
information about biologically interesting peptide-like antibiotic and inhibitor molecules in the PDB archiv



Automatic extraction from specialised databases

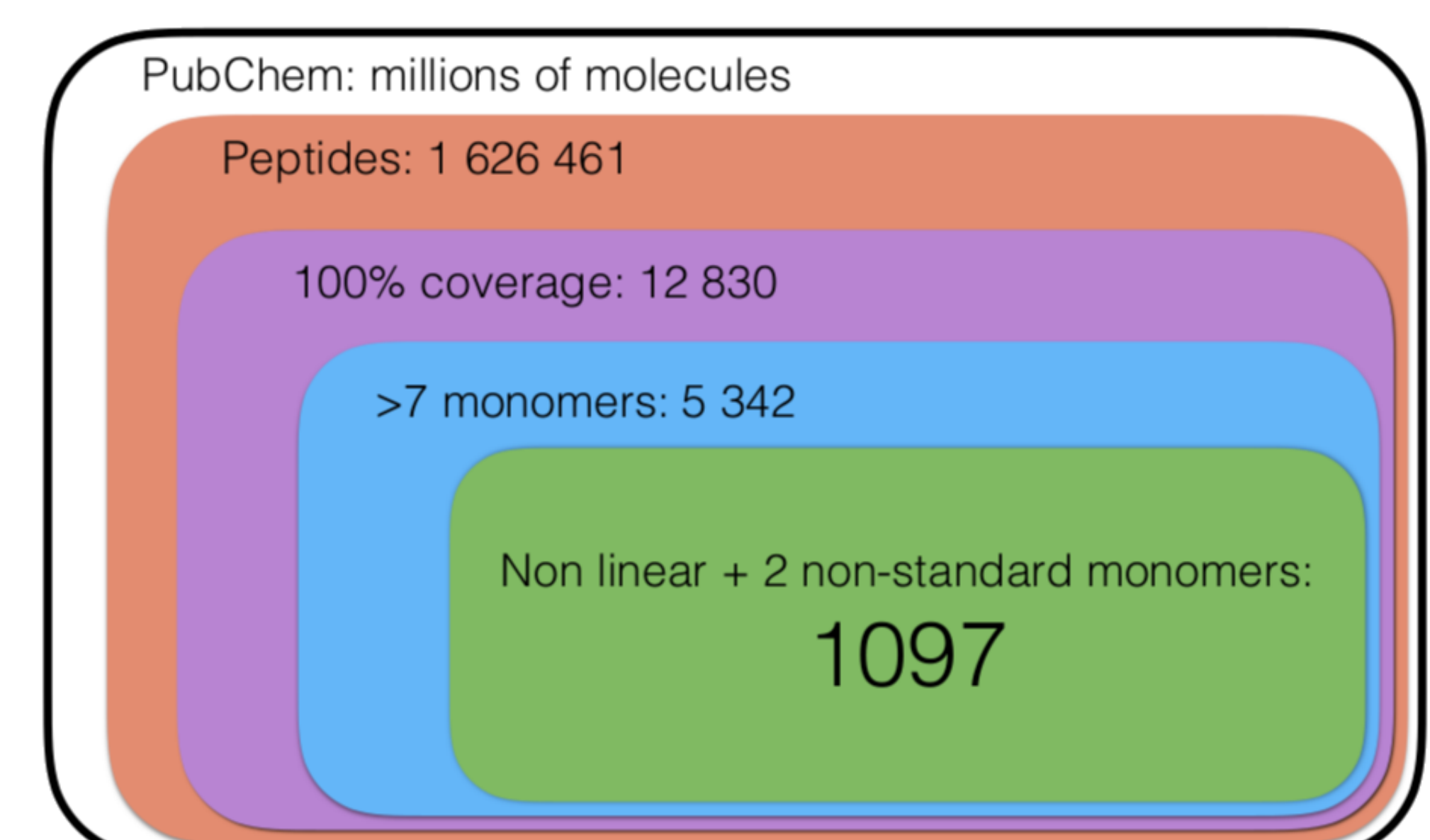
We develop scripts to extract known NRPs and fill up Norine

+472 NRP

Norine V3

Norine V3
1658 NRP

- +30% NRP
- Better quality than ever
- s2m to correct error before its appened



Proof of concept to screen chemical databases

- PubChem contains many NRPs but they are not annotated
- We use s2m to annotate their structures and then detect NRP candidates

Structure error detection

- 109 inconsistencies between the monomeric structures stored in Norine and the ones predicted by s2m from atomic structures.
- 20 have been manually corrected until now.

If I'm not in front of this poster and you want to contact me / you have questions :

Yoann Dufresne
mail : yoann.dufresne@unige.ch
phone : +33 (0)6 30 97 23 49

